

LA-UR-19-30027

Approved for public release; distribution is unlimited.

Title: Recent Advances in Monte Carlo Methods at Los Alamos National Laboratory

Author(s): Trahan, Travis John

Intended for: University seminar for recruiting

Issued: 2019-10-03

Disclaimer:

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by Triad National Security, LLC for the National Nuclear Security Administration of U.S. Department of Energy under contract 89233218CNA000001. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.



Delivering science and technology
to protect our nation
and promote world stability



Operated by Triad National Security, LLC for the U.S. Department of Energy's NNSA

Recent Advances in Monte Carlo Methods at Los Alamos National Laboratory

**Seminar for the Nuclear Engineering and Radiological
Sciences Department
University of Michigan**



Travis Trahan, XCP-3

October 3, 2019



Operated by Triad National Security, LLC for the U.S. Department of Energy's NNSA

Outline

- **Overview of XCP-3 and XCP-7:
Radiation Transport Codes/Applications**
- **Summary of Ongoing R&D in XCP-3**
- **Transient Reactor Analysis**
- **Stochastic Systems Analysis**
- **Tally Algorithms and Libraries for Advanced Computing Architectures**

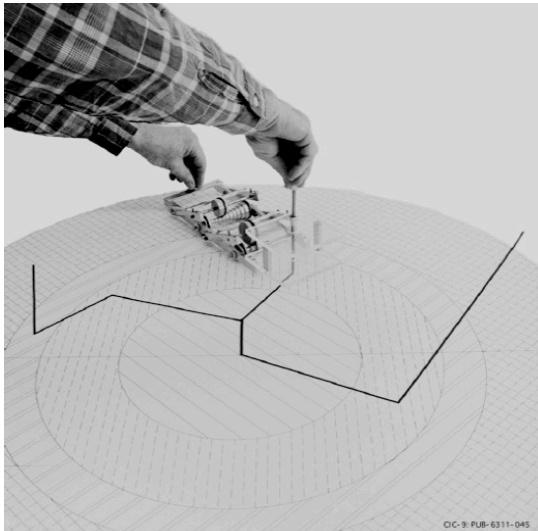
Overview of XCP-3 and XCP-7: Radiation Transport Codes/Applications

What is Monte Carlo Radiation Transport?

- **In general, Monte Carlo methods simulate large numbers of random trials in order to observe numerical behavior of systems described by probabilistic behavior**
 - Buffon's needle experiment to calculate π
 - Average and standard deviation of long term stock market returns
- **In radiation transport, pseudo-random number generators are used to randomly sample individual particle lives**
 - Source position, direction, and energy
 - Distance to collision
 - Collision type
 - Outgoing particle states
 - Repeat for many particle histories until each history ends (e.g., by leakage)
- **Information about the particles are tallied**
 - Reaction rates
 - Energy deposition
 - Multiplication

LANL's Long History with Monte Carlo

- **Monte Carlo Method for Radiation Transport Originated at LANL**
 - Stanislaw Ulam, John von Neumann, Robert Richtmyer, and Nicholas Metropolis
 - Early calculations performed on the FERMIAC11 and MANIAC machines
- **Monte Carlo code development and applications have been an important part of LANL efforts since that time**



FERMIAC11 mechanically traced neutron paths

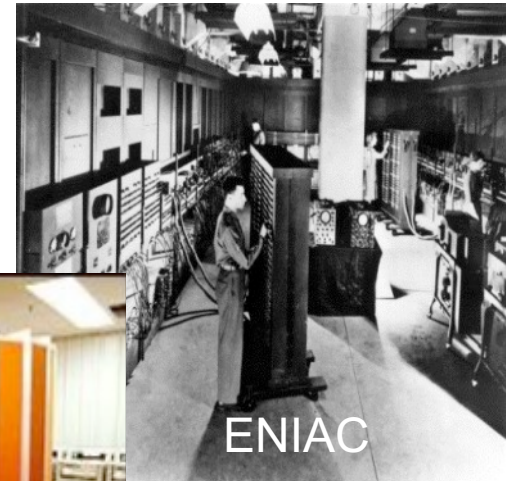


MANIAC computer performed early Monte Carlo calculations

History of Scientific Computing at LANL

Manhattan Project (1940's)

- **1945: ENIAC**
 - The first general purpose electronic digital computer
 - Built at University of Pennsylvania, but first used by LANL to study the hydrogen bomb



Cold War (1950's to 1992)

- **1953: IBM 701/704**
 - First programs stored in core memory
- **1965: CDC Model 6600**
 - The first supercomputer, first to use instruction pipelining
 - Up to 3 megaflops
- **1976: CRAY 1**
 - First successful vector machine
 - 160 megaflops



Science based stockpile stewardship (1992 to Present)

- **2008: Roadrunner**
 - Hybrid computer; first to break the petaflop barrier
- **2015: Trinity**
 - Half Haswell, half KNL
- **2021: Crossroads**



XCP-3/7: Radiation Transport Codes/Applications (Formerly Monte Carlo Methods, Codes, & Applications)

- **We deliver:**
 - First-principles Monte Carlo methods
 - Production-quality codes
 - Radiation transport-based computational and experimental assessments
- **Our codes (Now XCP-3):**
 - MCNP
 - MCATK
- **Our applications (Now XCP-7):**
 - Criticality safety
 - Non-proliferation
 - Nuclear energy
 - Nuclear threat reduction and response
 - Radiation detection and measurement
 - Radiation health protection
 - Stockpile stewardship

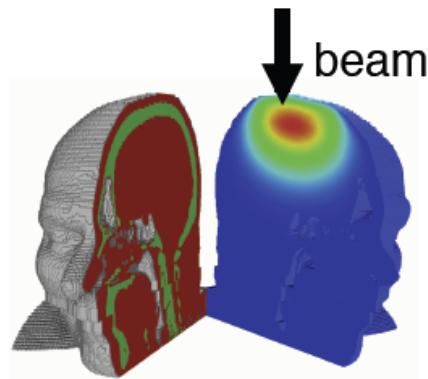
MCNP

- Decades of development and V&V have made it one of the most trusted radiation transport tools in the world
- Its key value is a predictive capability that can replace expensive or impossible-to-perform experiments
- Approximately 8000 copies of MCNP6 and 12000 copies of MCNP5 have been distributed



MCNP Won 2015 Richard P. Feynman Innovation Prize

CT geometries used for medical treatment planning



HEU-MET-THERM-003

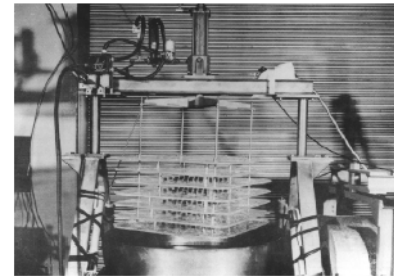
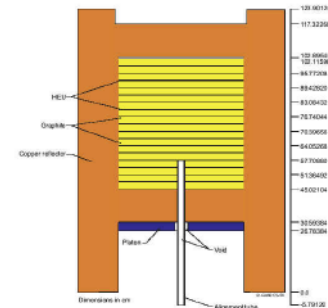


Figure 2. Array of 0.5-in. Cubes Prior to Immersion.

Zeus-2, HEU-MET-INTER-006, case 2



MCNP is validated against many criticality experiments

MCNP is the principle simulation tool of choice when the best answers are mandatory

MCNP

- **Physics:**

- Continuous energy particle transport
- Neutron, photon, electron, and many more particle types

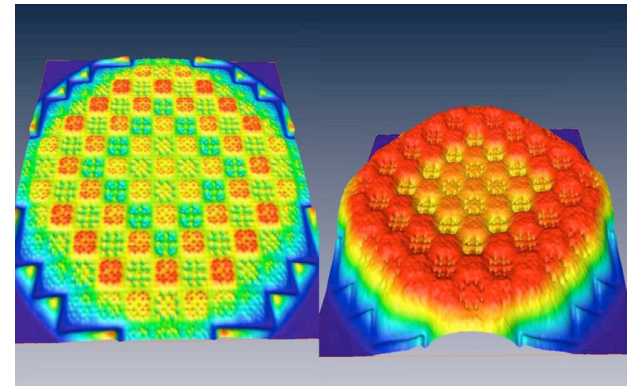
- **Algorithms:**

- k-eigenvalue calculations
- Fixed source calculations

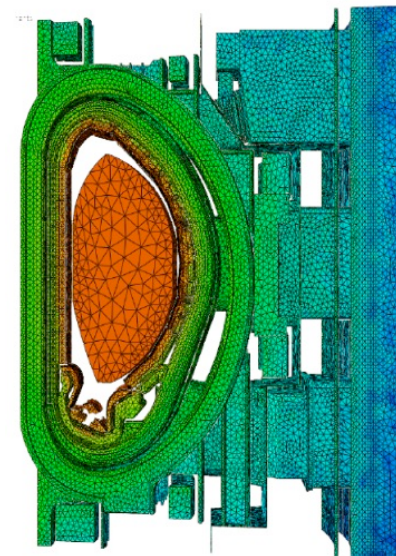
- **Recently Implemented Features:**

- Unstructured mesh transport
- Electric and magnetic field transport
- High-energy physics models
- 33 additional particle types
- Reactor fuel depletion and burnup
- Radiation source and detection capabilities
- Sensitivity and uncertainty analysis for nuclear criticality safety

Whole-core Thermal & Total Flux from MCNP5 Analysis
(from Luka Snoj, Jozef Stefan Inst.)



ITER Neutron Flux Calculations



MCNP Supporting Capabilities

- **CGMF – Correlated fission emission physics (XCP-3 POC: M. Rising)**
 - Most Monte Carlo codes use uncorrelated emission physics (e.g., average multiplicity); this is correct on average but incorrect on an event-by-event basis
 - Measurement of special nuclear material requires correct event-by-event knowledge
 - Samples fission fragments from each fission event and then uses Monte Carlo to sample each step during de-excitation of each fragment

Induced Fission Neutron Multiplicities for Plutonium-239

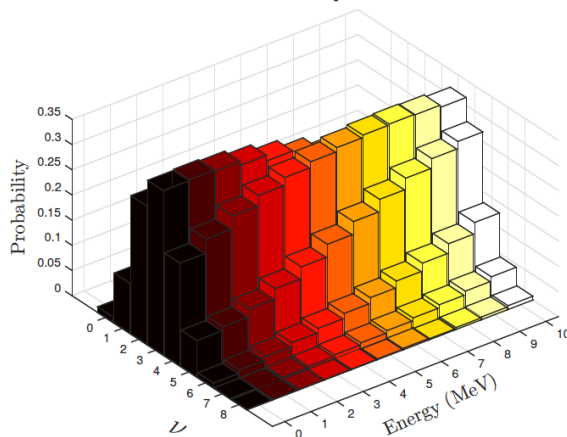
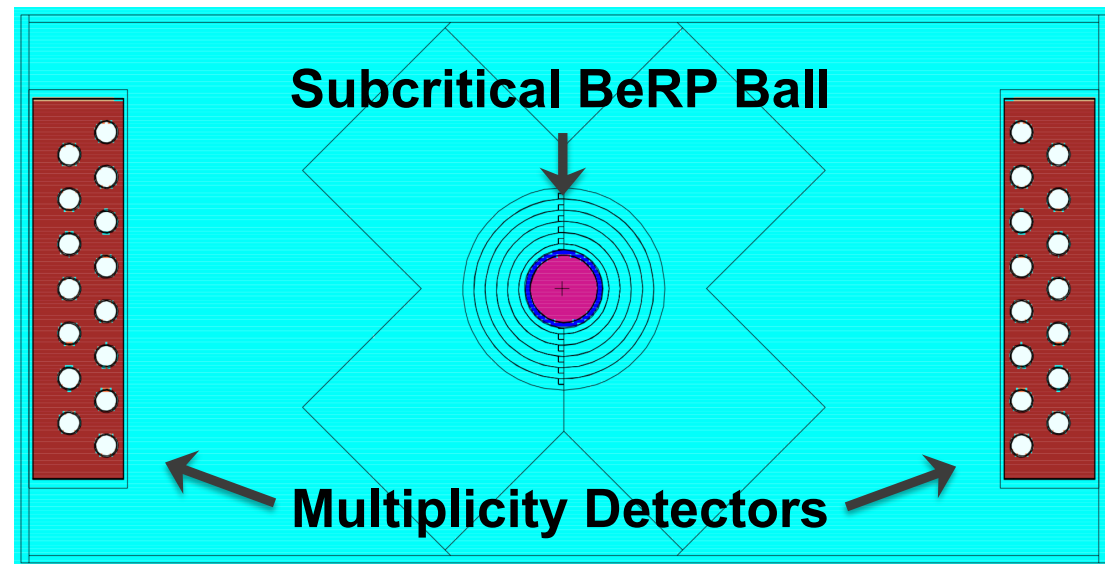


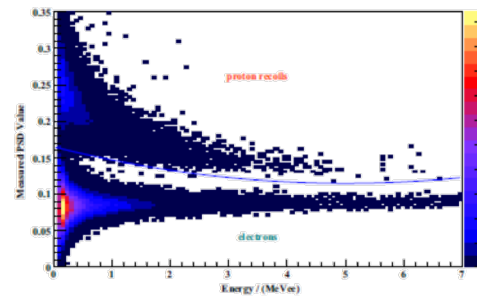
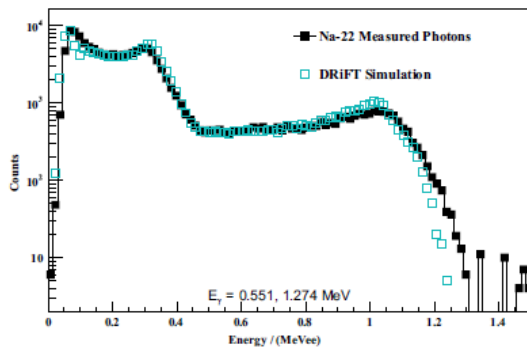
Figure taken from: M. Ortega, M.S. Thesis, University of New Mexico, NM.



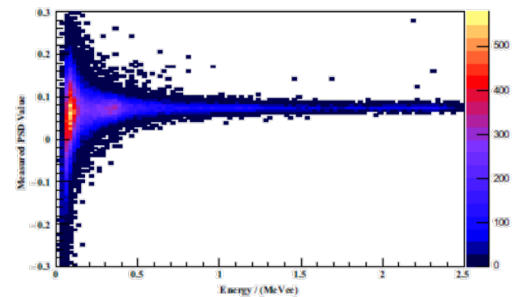
MCNP Supporting Capabilities

- **DRiFT – Detector Response Function Toolkit (XCP-7 POC: M. Andrews)**

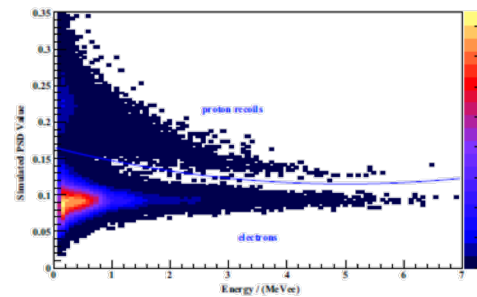
- MCNP has some detector features, but more are needed to properly simulate nuclear instrumentation
- DRiFT post-processes MCNP output and creates realistic detector responses
- Scintillators are most developed, gas detector and semiconductor physics are earlier in development



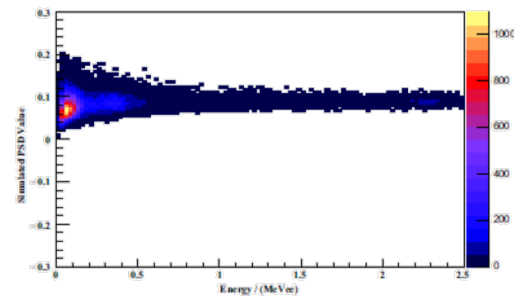
(a) Measured ²⁵²Cf



(a) Measured



(b) DRiFT ²⁵²Cf



(b) DRiFT

MCNP Supporting Capabilities

- **Intrinsic Source Constructor (ISC) (XCP-3 POC: J. Kulesza)**
 - Generate intrinsic radiation sources for inputs into transport codes
 - MISC: MCNP Intrinsic Source Constructor, generates SDEF distributions
 - Materials can be aged using built in Bateman solver
- **MCNPTools (XCP-3 POC: J. Kulesza, XCP-7 POC: C. Bates)**
 - Library that provides object-oriented access to MCNP outputs:
 - MCTAL files
 - MESHTAL B (MCNCP5 style) files
 - PTRAC files
 - LNK3DNT files
 - Python and Perl bindings provide an interface to load an output file and query it (e.g., `GetValue(I,J,K,E,T)` returns the tally value for the (I,J,K)th element for energy bin E and time bin T)

Monte Carlo Application ToolKit (MCATK)

- **C++ component-based Monte Carlo transport library**
 - Development began in 2008
- **Component-based means developing reusable components for:**
 - Building specialized applications
 - Provide new functionality in existing general purpose Monte Carlo codes like MCNP
- **Developed with modern software engineering methodologies:**
 - Agile development: Incremental development cycles
 - Pair programming: Improves design and testing, sharing of code knowledge reduces technical debt
 - Test driven development: Unit testing and integrated physics testing for verification and validation

MCATK is a suite of tools intended to enable rapid development and deployment of custom Monte Carlo solutions

MCATK

- **Physics:**

- Continuous energy particle transport
- Neutron-photon only (for now)

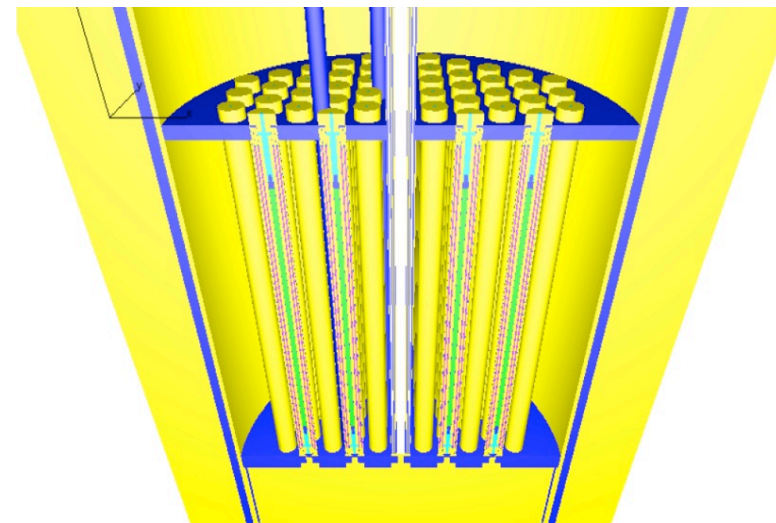
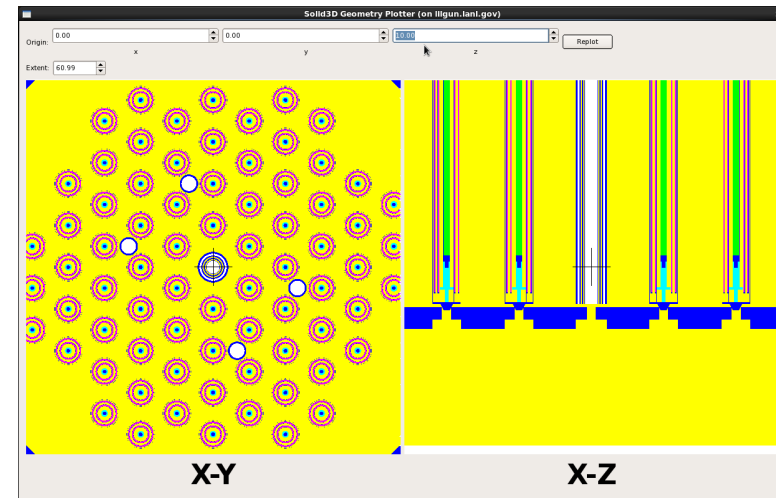
- **Algorithms:**

- k- and α -eigenvalue calculations
- Fixed source calculations
- Time-dependent calculations
- Fission chain analysis

- **Recently Implemented Features:**

- Solid body geometries
- Visualization Tools
- Expanded source options
- Expanded tally types
- Weight-windows
- Python interface for problem setup
- Additional fission chain analysis algorithms

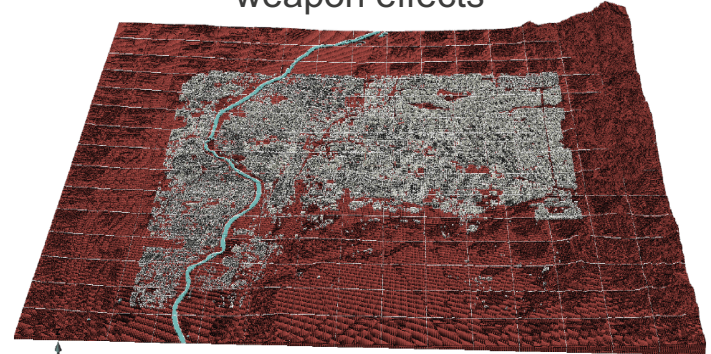
MCATK solid body representation of
ICT2C3 Critical Benchmark



XCP-7: Radiation Transport Applications

- Radiation detection, simulation, and measurements
- Nuclear diagnostics simulations
- Intrinsic radiation
- Emergency response / nuclear threat assessments
- Nuclear weapon effects and outputs (e.g., EMP)
- Criticality safety
- High energy physics

City model used to study nuclear weapon effects



XCP-3 / NEN-2 staff make measurements and use MCNP6 to help design neutron shielding on the next generation of Ohio-class nuclear submarine



Applications staff work across groups and in the field performing both simulations and measurements in support of national security

Summary of Ongoing R&D in XCP-3

XCP-3 at M&C 2019

T.P. Burke, C.J. Josey , B.C. Kiedrowski, “Monte Carlo Estimates of Alpha-Eigenvalue Sensitivities via Differential Operator Sampling”	F.B. Brown, C.J. Josey , S.J. Henderson, W.R. Martin, “Automated Acceleration and Convergence Testing for Monte Carlo Criticality Calculations”
C.J. Josey, F.B. Brown , “Stabilizing the k-Alpha Iteration Algorithm in Very Subcritical Regimes”	D.H. Timmons, M.E. Rising , C.M. Perfetti, “The Use of MCNP 6.2 KCODE for High Fidelity, Near Critical Benchmarks”
P. Grechanuk, M.E. Rising , T.S. Palmer, “Identifying Sources of Bias from Nuclear Data in MCNP6 Calculations Using Machine Learning Algorithms”	S.R. Bolding , A.R. Long, K. Beyer, K.P. Keady, “A Fully Monte Carlo Solution of the Thermal Radiative Transfer Equations with Compton Scattering”
B. Whewell, R.G. McClarren, S.R. Bolding , “Data Fusion Techniques for Improving Fission Neutron Multiplicity Data”	G. Giudicelli, W. Wu, C.J. Josey , B. Forget, K.S. Smith, “Adding a Third Level of Parallelism to OpenMOC, an Open Source Deterministic Neutron Transport Solver”
B.C. Kiedrowski, J.A. Kulesza , C.J. Solomon, “Discrete Ordinates Prediction of the Forced-Collision Variance Reduction Technique in Slab Geometry”	J.A. Kulesza , C.J. Solomon, B.C. Kiedrowski, “Predicting Monte Carlo Tally Variance and Calculation Time when using Forced-flight Variance Reduction-Theory/Verification” (Two Talks)
T.J. Trahan , “Monte Carlo Calculations of the Burst Wait Time of Fast Burst Reactors Using MCATK”	C.J. Josey, F.B. Brown , “Computing Alpha Eigenvalues Using the Fission Matrix”

XCP-3 publishes an impressive amount of research

Static Alpha Eigenvalue

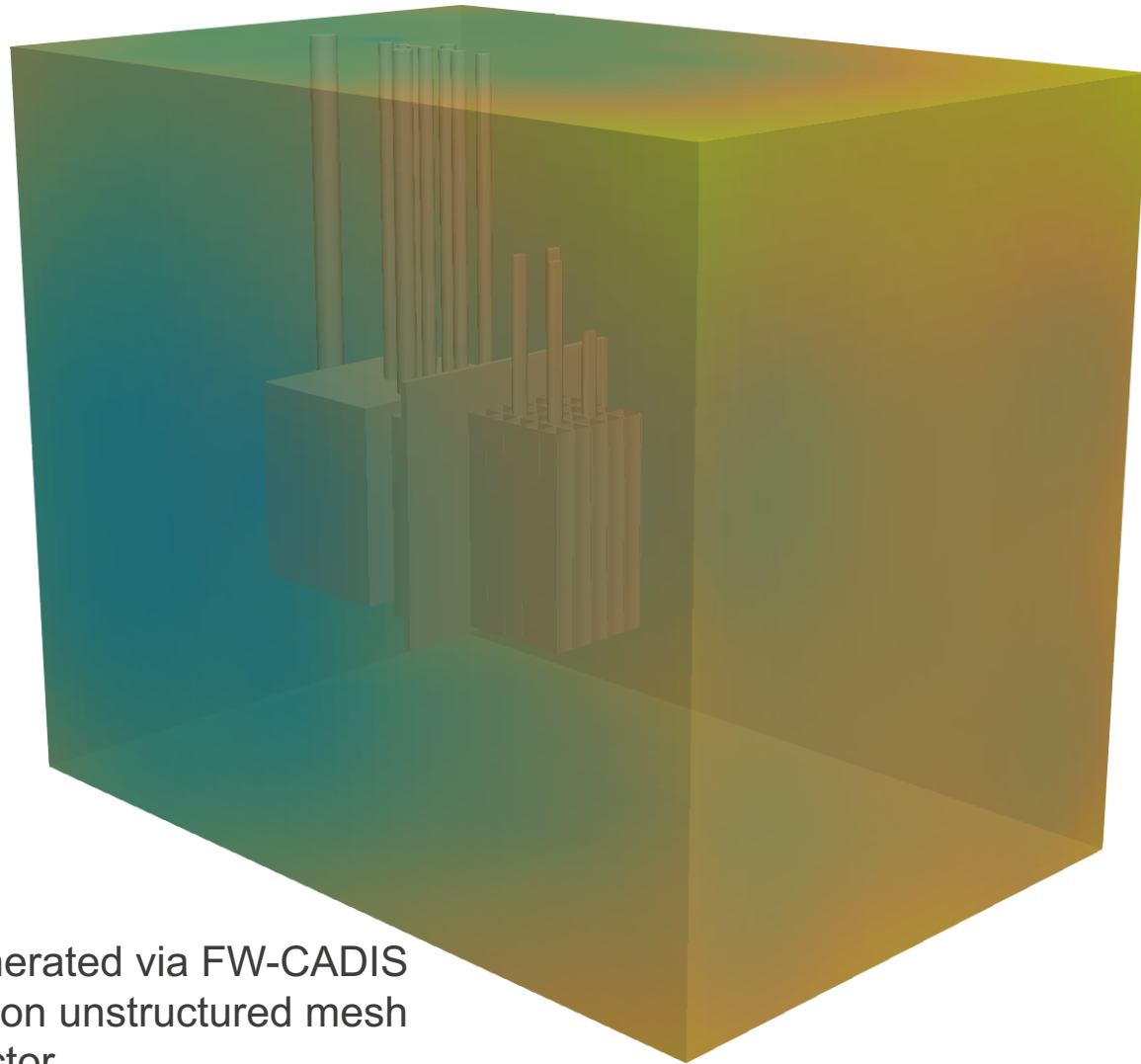
- **Improved k-alpha eigenvalue solver in MCNP**
 - Previously, updated guesses of alpha based on the value of k
 - Now, update alpha based on a few tallies over all phase-space during each generation
- **Stabilization of the k-alpha iteration in very subcritical regimes**
- **Calculation of alpha using a time-dependent fission matrix**
- **Calculating sensitivity of alpha via differential operator sampling**

Automated Acceleration and Convergence Testing for Monte Carlo Criticality Calculations

- **Eliminates the need for users to perform scoping runs and assess Shannon entropy plots manually**
- **Based on tallying a fission matrix**
 - Mesh spacing and extents are adaptively determined
- **Statistical tests on k and the fission matrix determine when the fission source is converged after blocks of cycles**
 - Fission source biasing is performed based on the fission matrix during inactive cycles
 - When k and the fission source are determined to be converged, automatically begin active cycles and stop biasing
- **Checks at the end of the simulation assess if the simulation used enough particles per cycle**

Variance Reduction

- **Prediction of run time and tally variance for different variance reduction techniques**
 - Attempt to optimize computational efficiency, not just minimize variance
- **Automated weight window generation by implementing FW-CADIS, Cooper-Larsen methods**



Weight-Windows Generated via FW-CADIS
in Advantg overlaid on unstructured mesh
geometry of pool reactor

- **Statistical testing**

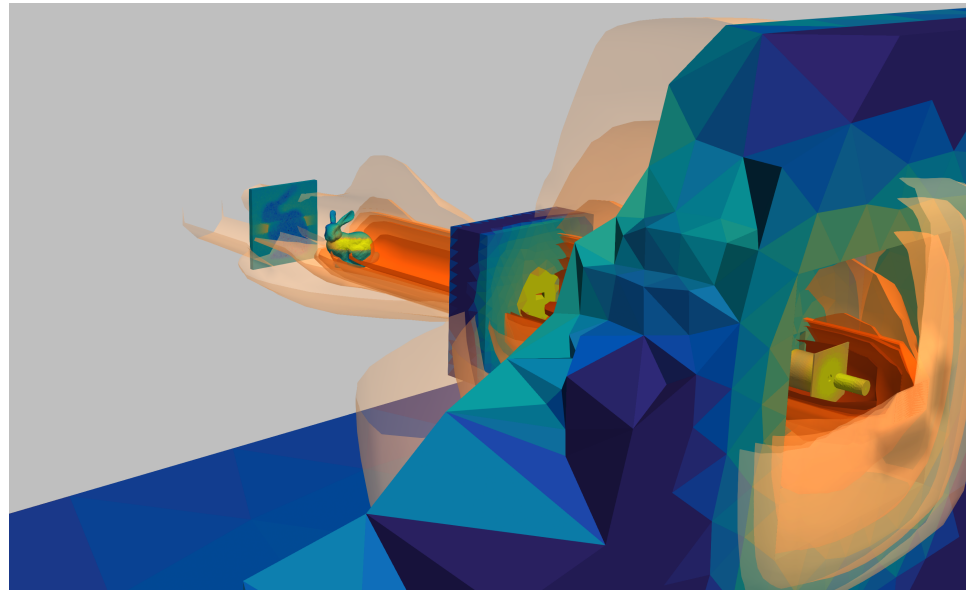
- Any change to a Monte Carlo code that changes the random number usage has the potential to break many regression tests
- Differences may be large compared to numerical precision, but still statistically identical; how do we know if there's a bug
- Creating a tool to assess changes in tally results so that we can change the code with confidence

- **Improving automated testing and reporting**

- **Always need to setup and run more benchmark tests, especially as we model new classes of problems or implement new features**

Modernization

- **Converting many output files to HDF5 (+XDMF in some cases)**
 - Runtape (complete)
 - EEOOUT (in review)
 - Mesh tally, tmesh (prototyped)
 - Ptrac
 - wwinp
- **Ptrac will soon run in parallel**
- **Modularization**
 - Make MCNP less monolithic
 - Rewrite modularized components as standalone libraries
- **Workshops are undergoing major revisions and those that have been completed have received positive reviews**

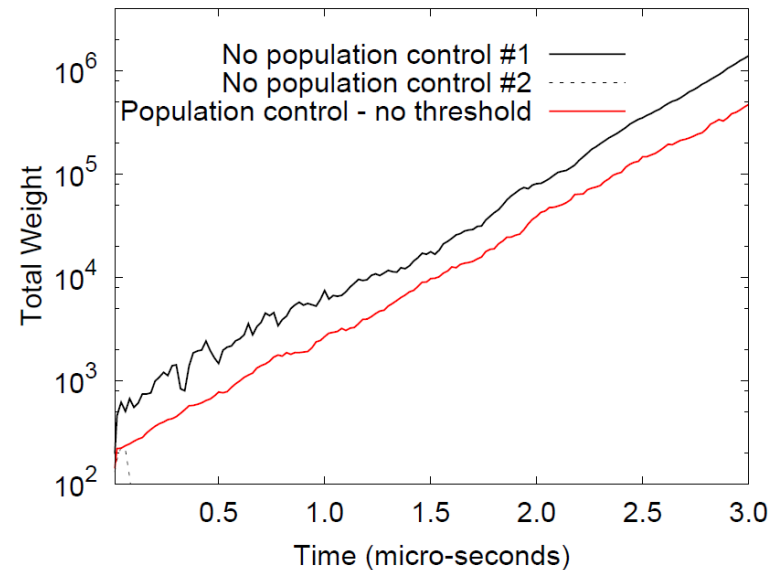


Stanford bunny in notional radiography facility using unstructured mesh and HDF5 output

Transient Reactor Analysis

Time-Dependent Algorithm

- Problems are driven by a user-defined, possibly time-dependent source
- Simulations are discretized in time
- When particles reach the end of a time step, they are added to a bank called the “census”
- Population control is applied between time steps
 - Maintains approximately the same number of samples in every time step
 - Enables modeling of sub- and super-critical problems
- Some of the codes that use this algorithm are: TART, Serpent, McCARD, MCATK



This algorithm is effective but computationally expensive due to the difference in time scales between neutron lifetime and the transient

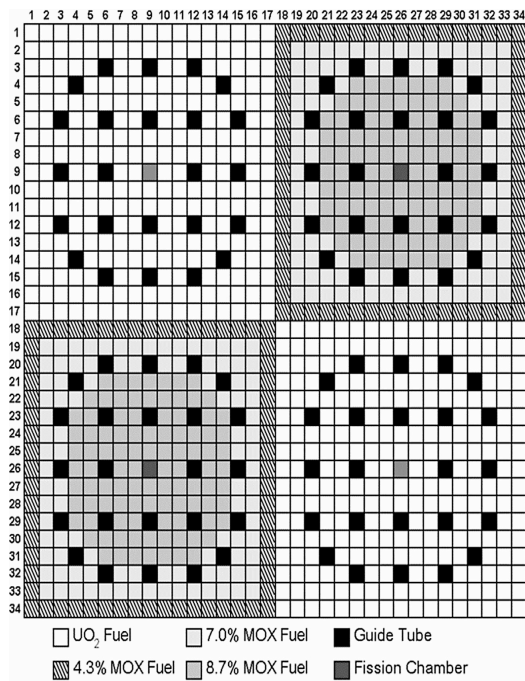
Delayed Neutron Treatments

- **Sampling delayed neutrons directly at each fission is infeasible:**
 - Delayed neutrons may be born seconds or minutes after fission, possibly after the transient
 - In the meantime, they must be stored in a constantly growing bank of particles
- **Instead, sample and store delayed neutron precursors (DNPs):**
 - The DNPs emit delayed neutron samples continuously, i.e., emit a fraction of their weight every time step
 - No wasted storage
 - Better statistics due to continuous emission
- **This kind of delayed neutron modeling used in B. Sjenitzer's Dynamic Monte Carlo method also used in McCARD and SERPENT**

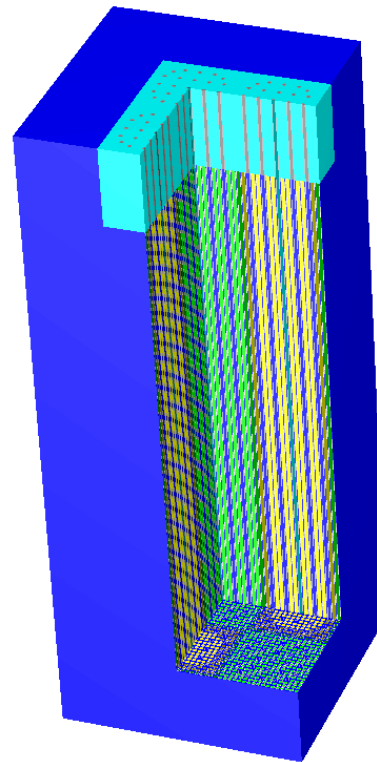
Sampling delayed neutron precursors instead of delayed neutrons saves memory and improves statistics

C5G7 Transient Benchmark

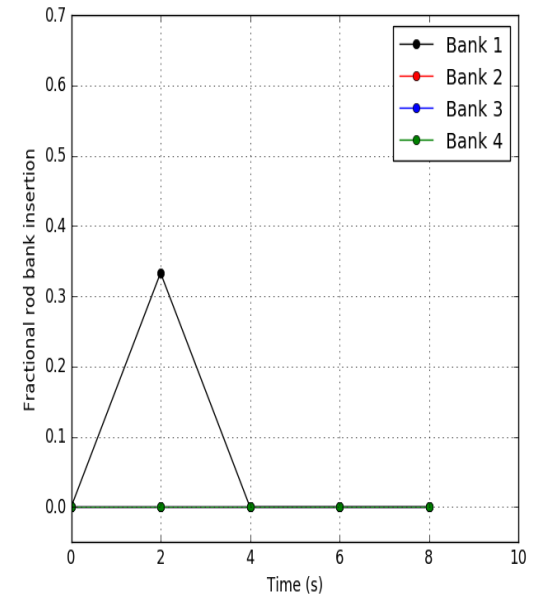
- Four assembly reactor (2 MOX, 2 UO₂)
- Control rod banks inserted from the top
- Using the continuous energy version of the benchmark EXCEPT using the multigroup delayed neutron emission spectra



Assembly Compositions



3D Configuration

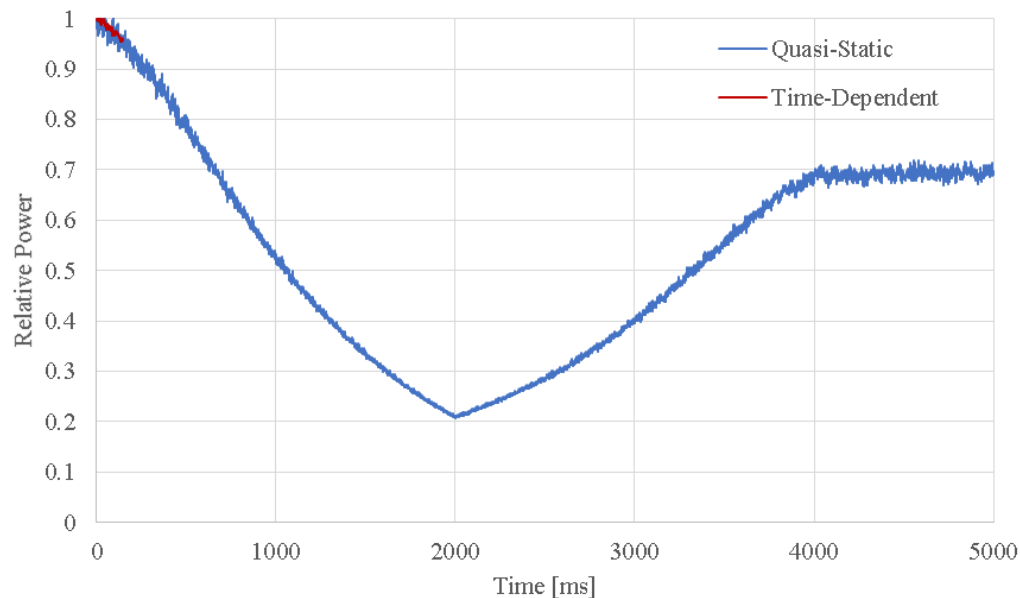


Transient Problem TD4-1

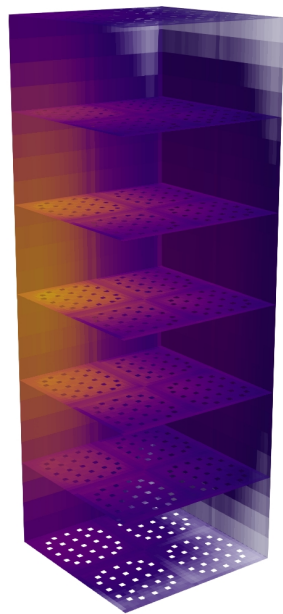
C5G7 Transient Benchmark Results

- Run quasi-static: 10 μs micro time steps, 1 micro step per macro step, 100 μs macro time steps
- Total powers are tallied every micro step
- 3-D Powers are tallied separately from the main calculation for 100 x 10 μs time steps
- NOTE: Power should rise slowly after 4s; the cause of the incorrect flat behavior is known but not yet fixed

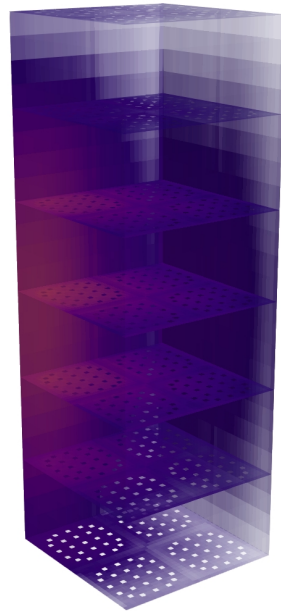
Need to rerun this with some changes: no prompt neutron census, longer time steps, separate population control for each DNP group



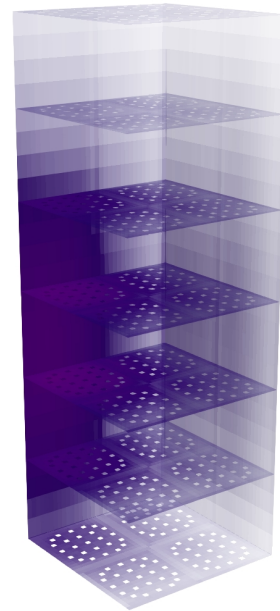
C5G7 Transient Benchmark Results



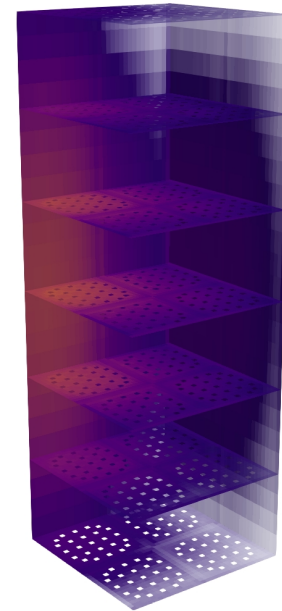
0 s



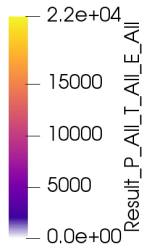
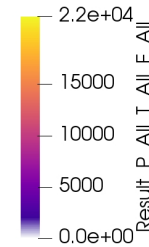
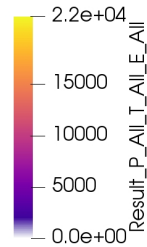
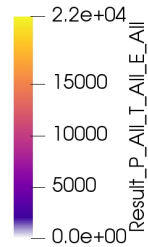
1 s



2 s



4 s

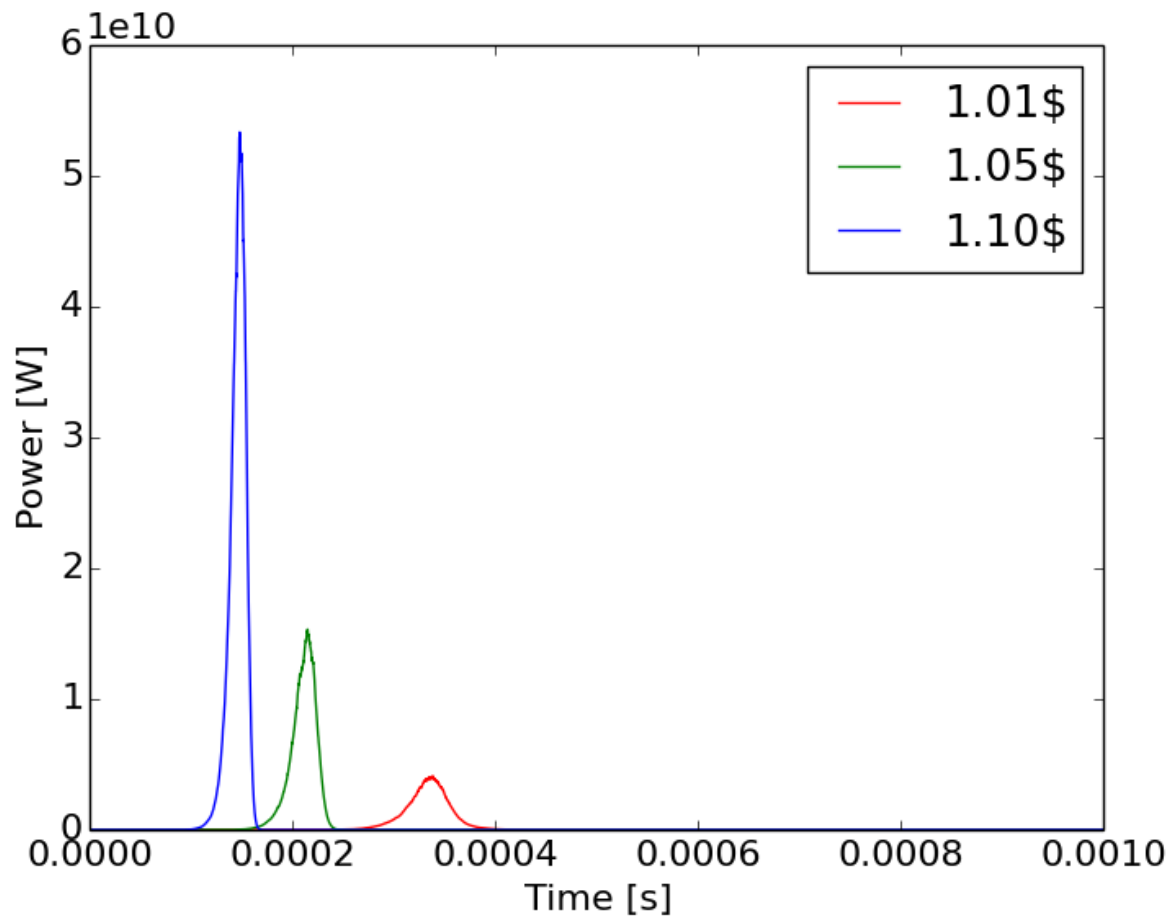


Multiphysics Simulations of Lady Godiva

- **MCATK has been coupled to simple 1-D thermomechanics solver**
- **Godiva is simulated using a pseudo-1-D domain.**
 - Neutron transport is done in 3-D.
 - Multiphysics is done over a 1-D, spherically symmetric domain.
- **Simulations are shown for \$1.01, \$1.05, and \$1.10 insertion reactivities.**
 - Temperature and density are initially uniform.
 - Mesh is initially undeformed.

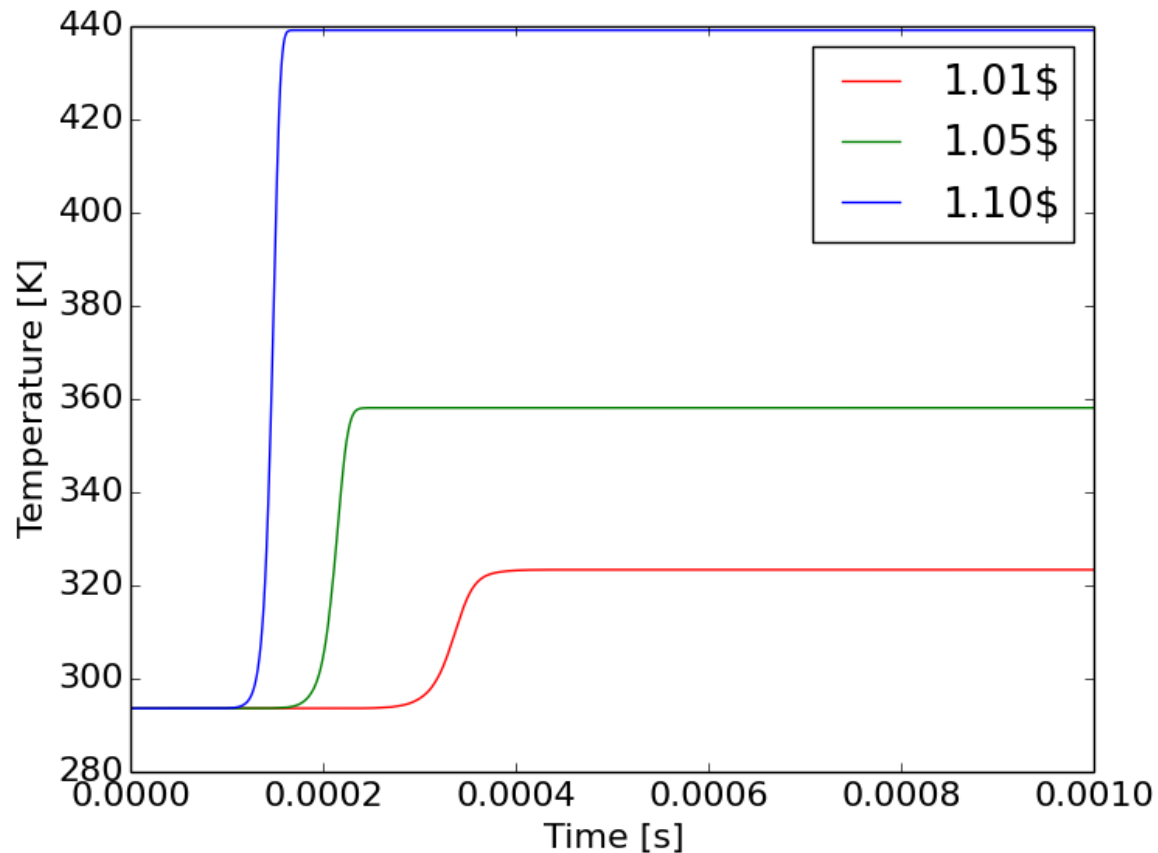
Results

- Prompt super-critical pulses elevate power output for a brief period.



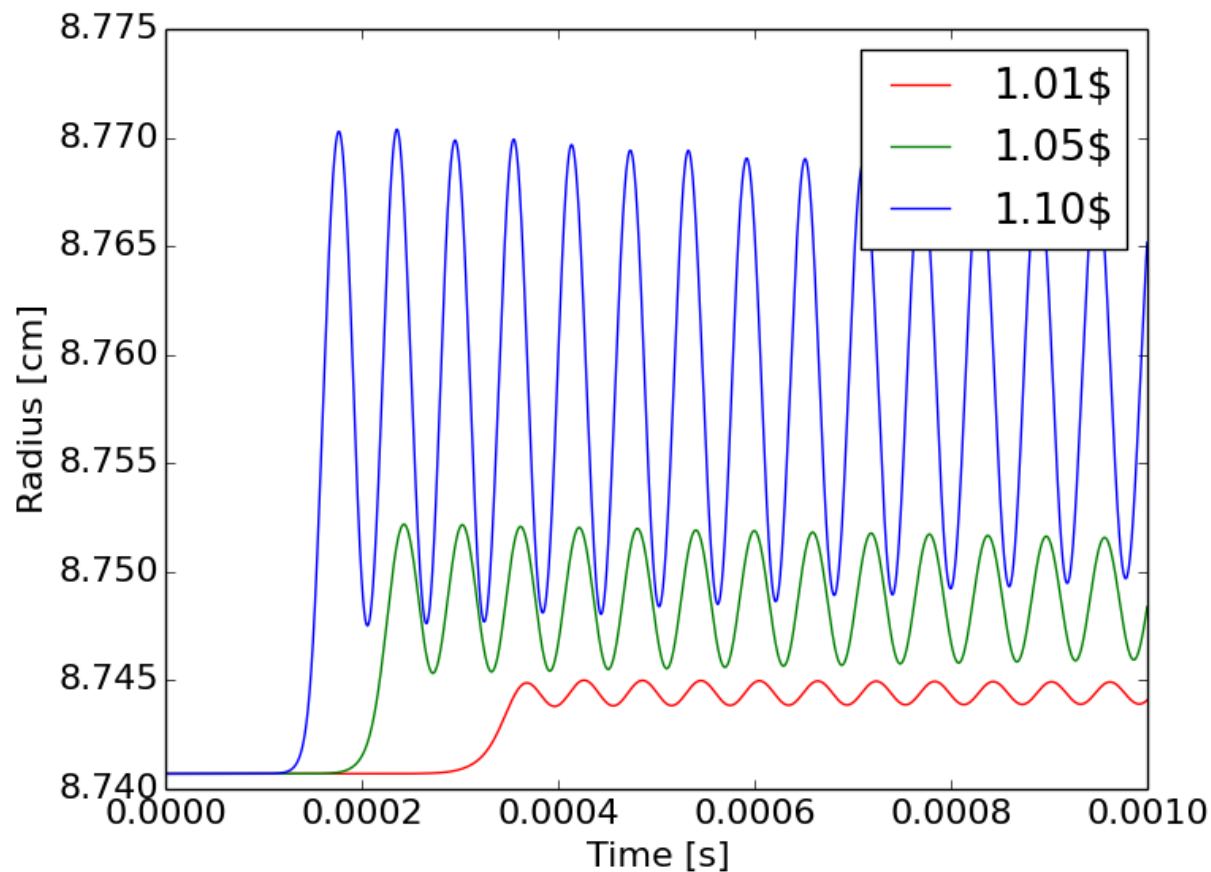
Results

- Average temperature rises due to neutron thermalization and remains constant due to assumption of no external radiation.



Results

- Once expansion due to rising temperatures has ceased, radial oscillations occur due to the assumption of a purely elastic medium.



Stochastic Systems Analysis

What are Stochastic Systems?

- **Stochastic Systems:**

- Contain weak sources and low neutron populations
- Contain fission chains that do not overlap
- May exhibit behavior that varies significantly from the expected or average behavior of the system

- **Examples:**

- Subcritical experiments
- Pulsed nuclear reactors (e.g., Godiva, Caliban)
- Criticality accident scenarios
- Fissile material measurements for safeguards/nonproliferation
- Reactor startups

Deterministic Analysis of Stochastic Systems

- **Deterministic methods for characterizing stochastic systems first developed by Bell**
- **Deterministic analysis has been implemented in PARTISN and PANDA**
- **Deterministic equations take the form of coupled adjoint transport equations with modified source terms**
- **Can calculate:**
 - Single particle probabilities of initiation / extinction / survival (POI / POE / POS)
 - Moments of the neutron and fission number distributions resulting from single neutrons or neutron sources.

Monte Carlo Analysis of Stochastic Systems

- **Simulate the random histories of complete fission chains from birth to extinction and observe their stochastic behavior**
- **Tally:**
 - Response, dose, or number of events (e.g., fissions, leakage) for every fission chain
 - Total / net / leakage multiplication
 - POI / POE / POS
- **POI capabilities have been implemented in Mercury, a research version of MCNP, and the Monte Carlo Application ToolKit (MCATK)**

Basic Elements of the Monte Carlo Fission Chain Algorithms

- **Each source particle gets an ID, which is inherited by all progeny to identify them as being a part of the same chain**
- **At any given time, we know:**
 - Total chain length
 - Instantaneous chain population
 - Total number of fission or leakage events
- **In principle, any standard tally can be accumulated on a chain-by-chain basis**
- **No load balancing in order to keep entire fission chains on a single process**

Static Analysis: Multiplication

- **Total Multiplication: Total neutrons produced per source neutron**

$$M_T = Avg(ChainLength)$$

- **Net Multiplication: Net neutrons produced per source neutron (excludes neutrons lost to fission and NXN reactions)**

$$M_N = Avg(ChainLength - NumChainFissions - NumChainNXN)$$

- **Leakage Multiplication: Number of neutrons that leak per source neutron**

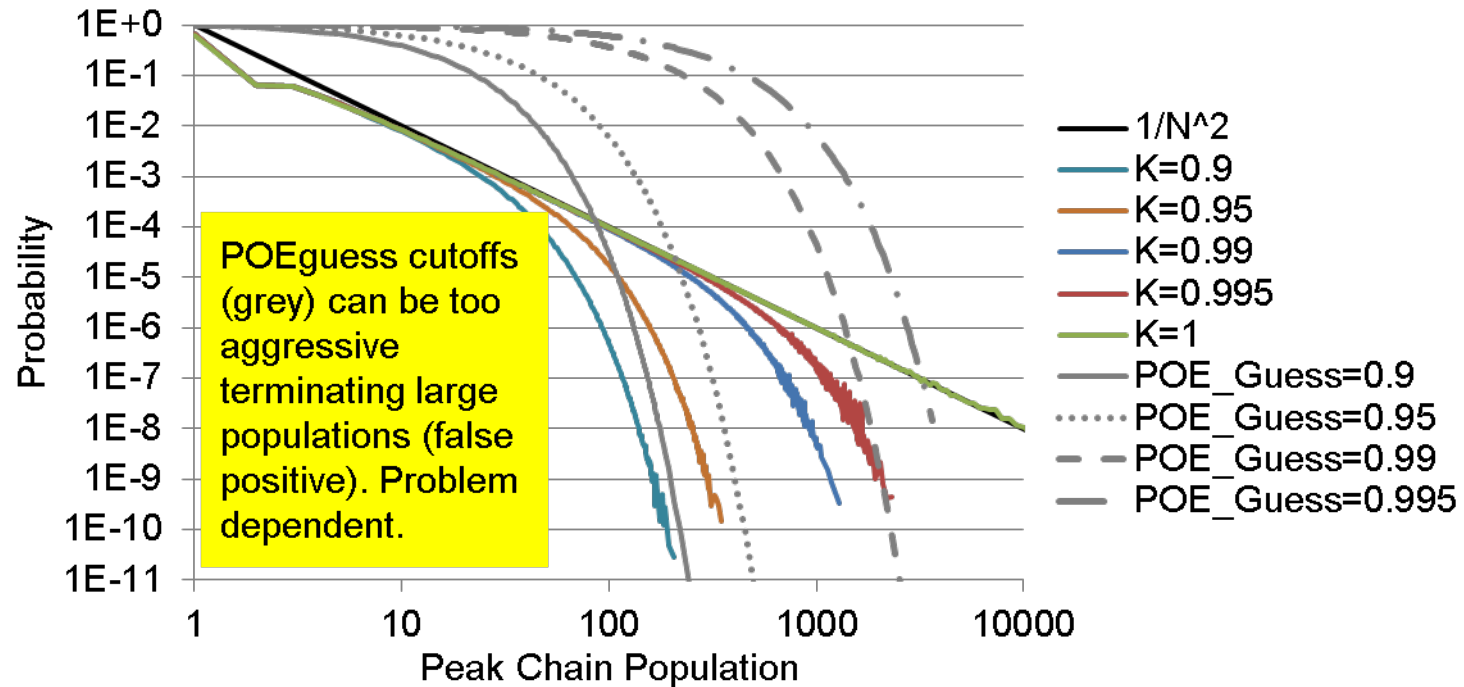
$$M_L = Avg(ChainLeakage)$$

Static Analysis: Probability of Initiation/Extinction

- **Probability of Initiation (1 - Probability of Extinction):** Probability that a fission chain persists for an infinite time, i.e., diverges
- **Cannot track an infinitely long chain, must terminate chains**
- **Cutoff method for POI:**
 - Specify a cutoff length or population above which a chain is terminated
 - Score the terminated chain to POI
 - Overestimation bias
- **Importance methods for POE:**
 - Give each chain an importance and a weight
 - Larger chains are less important to POE
 - Play Russian Roulette on entire fission chains

Static Analysis: Probability of Initiation/Extinction

- **Booth Importance:** $I = \frac{1}{(POE_{Guess})^{N-1}}$
- **“N Left” Importance:** $I = \frac{C}{N^2}$

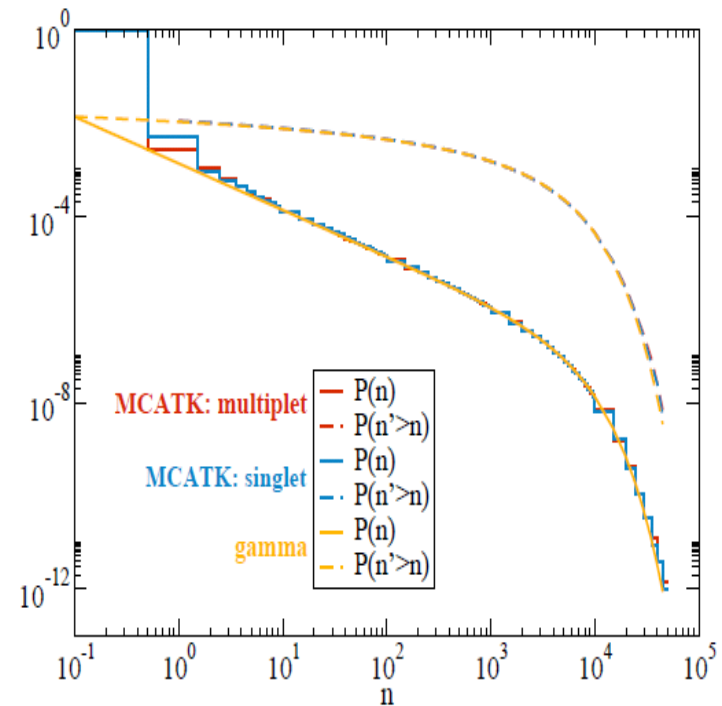


Dynamic Analysis

- We are interested in fission chain behavior over the entire transient, so we cannot terminate chains
- We do not want chains to grow too large (memory constrained), but we do want to allow them to become small and die off
- Algorithm summary:
 - Initially, track all chains in an analog fashion
 - When the chain population exceeds a threshold, *apply population control on a chain-by-chain basis*
 - Can roulette if the chain grows, or split if the chain shrinks
 - If the average weight of particles in the chain drops below the initial source particle weight due to splitting, track analog again

What is the Neutron Number Distribution?

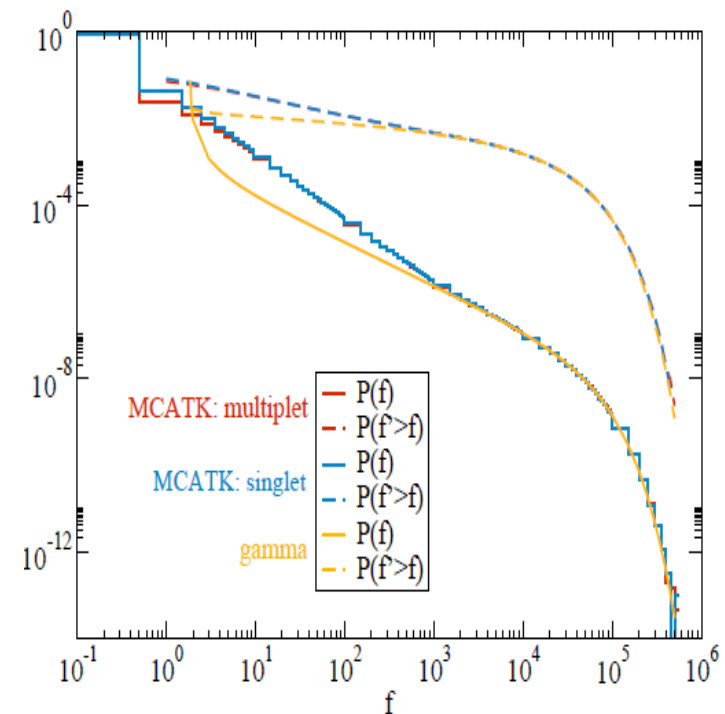
- The number of neutrons in the system is a stochastic quantity
- Imagine performing a measurement of the number of neutrons many times
- Calculate the probability of the system containing (0, 1, 2, ...) neutrons at some instant in time
- For a stochastic system, these distributions are non-normal with long tails towards larger numbers
- Distributions can be characterized by their moments (mean, standard deviation, skewness, and kurtosis)



Work performed by Erin Davis (LANL)

What is the Reaction Number Distribution?

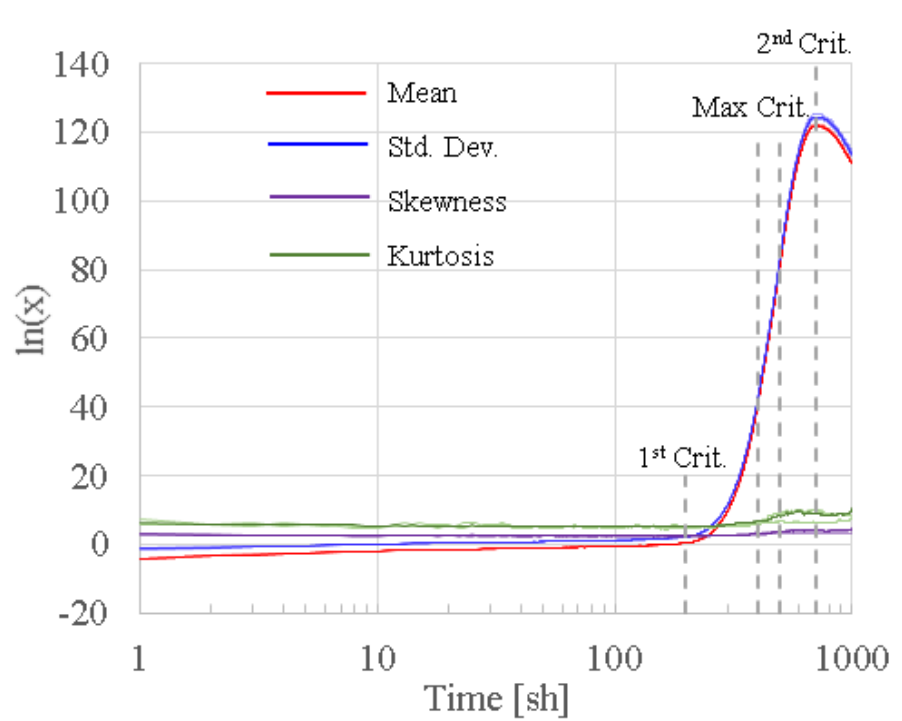
- Similar to the neutron number distribution
- Count the cumulative number of events of a certain reaction type up to some instant in time
- Calculate the probability of (0, 1, 2, ...) reactions occurring up to that instant in time
- Distributions can be characterized by their moments (mean, standard deviation, skewness, and kurtosis)



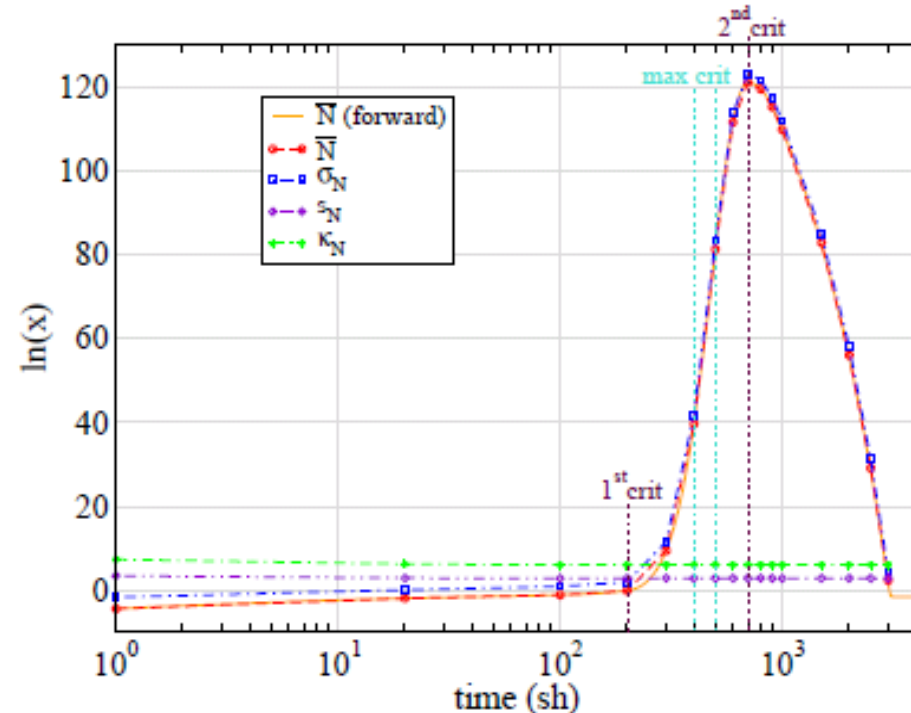
Work performed by Erin Davis (LANL)

Fission and Neutron Number Distributions for Uranium Sphere with Time-Varying Enrichment

Uranium sphere starts subcritical, transitions to supercritical, then transitions back to subcritical by artificially changing enrichment



MCATK

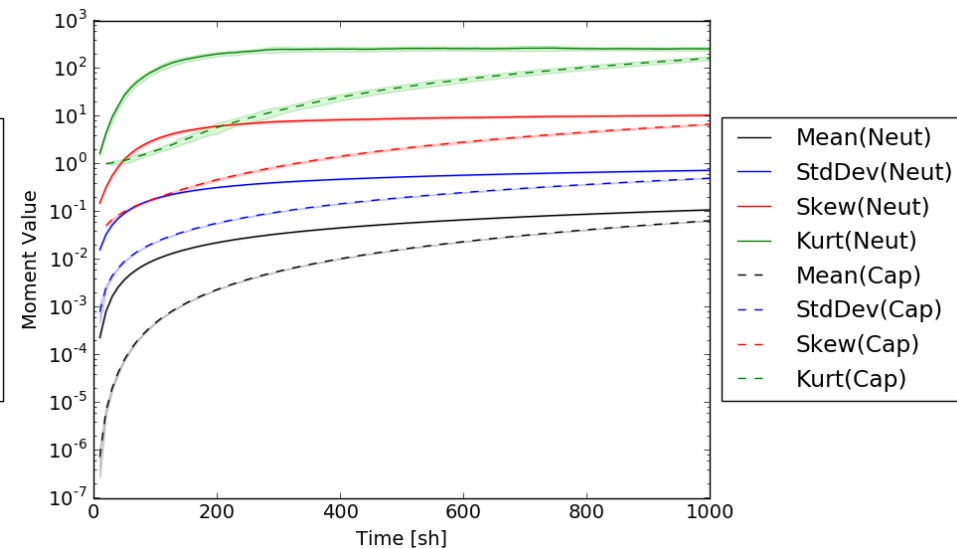
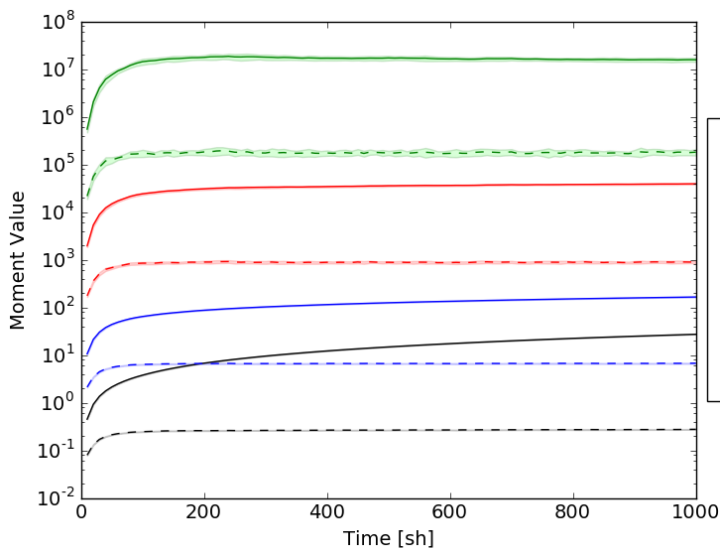


PARTISN

The deterministic and Monte Carlo approaches to calculating these moments are vastly different but yield the same result.

Region-Specific Moments for a Plutonium Sphere Surrounded by Polyethylene-Moderated He-3 Detectors

Plutonium sphere surrounded by four polyethylene-moderated He-3 detectors, each with a different reflector thickness



Moments of the Neutron Number in the Full System and Limited to the Plutonium Sphere.

Moments of the Neutron and Capture Numbers in Detector Number 3 (5.0 cm HDPE Moderator).

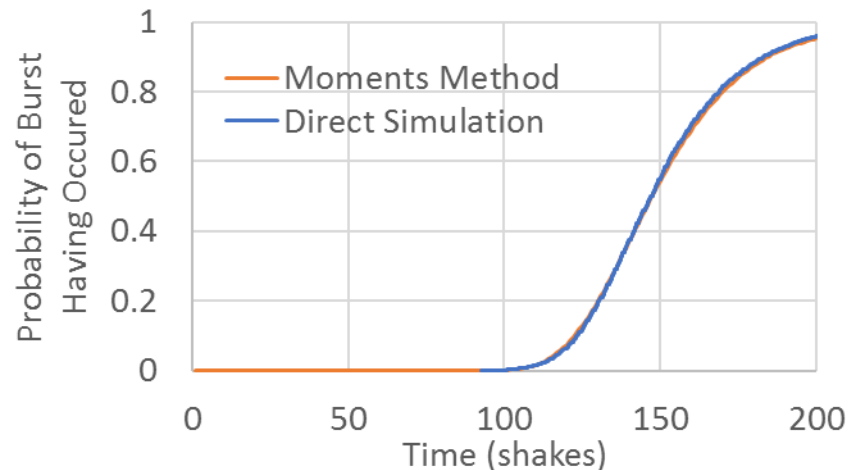
Looking at the moments for an entire system could be misleading since behavior in detector regions may be very different.

What is Burst Wait Time?

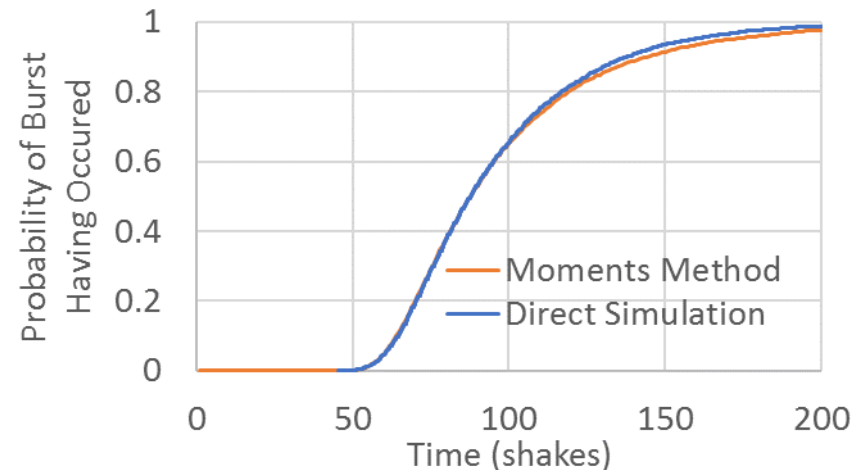
- Time between the insertion of reactivity into a fast burst reactor and the time at which the burst actually occurs
- Due to random timing of spontaneous fission events and the fact that many fission chains will die out before a burst, the burst wait time of a single experiment is randomly distributed
- Without an external neutron source, this delay can be on the order of seconds

Burst Wait Time: Direct Simulation vs. Moment Method

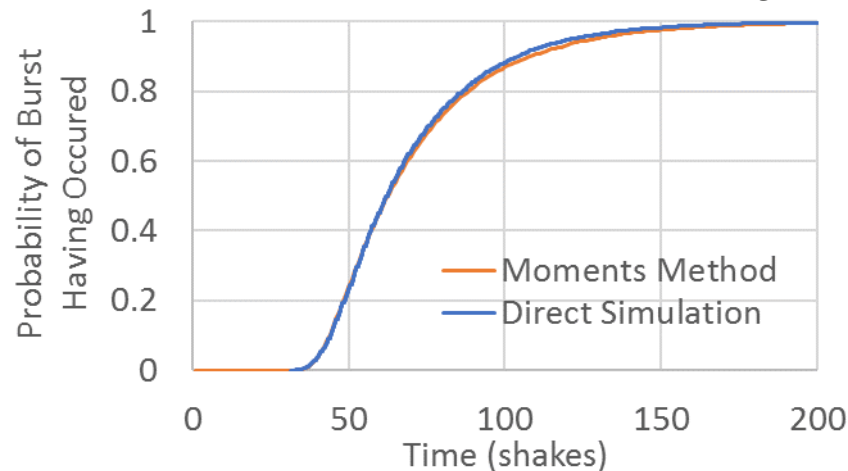
Three slightly supercritical plutonium spheres



5.1 cm Pu, $K_{eff} = 1.0112$



5.2 cm Pu, $K_{eff} = 1.0284$



5.3 cm Pu, $K_{eff} = 1.0434$

These simulations
performed by Kevin
Hase, XCP-7

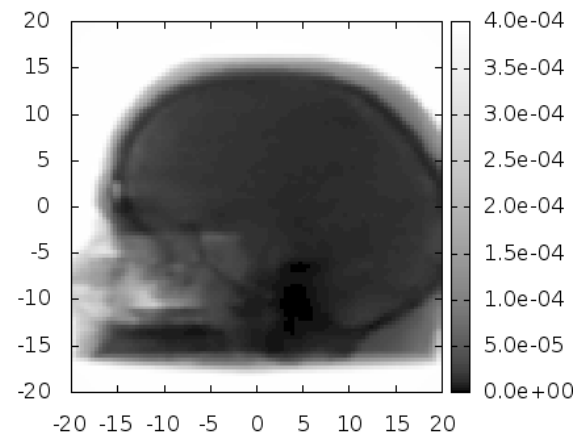
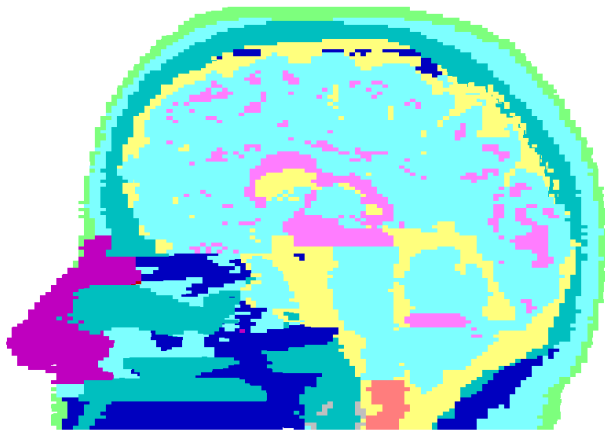
Tally Algorithms and Libraries for Advanced Computing Architectures

Why are Advanced Architectures Challenging for Monte Carlo?

- **Advanced architectures often use Graphics Processing Units (GPUs)**
- **GPUs are especially common**
 - GPUs have thousands of threads organized into groups called “warps”
 - Every thread in a warp must execute the same commands; “thread divergence” within a warp significantly decreases performance
 - Data must be transferred back-and-forth between CPU and GPU
 - GPUs have significantly lower memory per core
 - Code must be compiled specifically for the GPU and often requires using special languages (e.g., CUDA)
- **Monte Carlo algorithms are not well suited for these architectures:**
 - Random behavior means thread divergence is ubiquitous; vector Monte Carlo algorithms are available but require significant rewriting of code
 - Continuous energy data and tallying are very memory intensive

MonteRay Tally Library

- XCP-3 POC: J. Sweezy
- Supports performing tallies on GPUs asynchronously with transport on CPUs
- Takes a list of rays from a Monte Carlo transport code and performs one of two tallies based on ray tracing:
 - Next event estimators (point detectors)
 - Volumetric-ray-casting estimator
- Intended for open-source distribution!



Simulated Radiograph of Human Head (15x performance)

Talon Tally Library

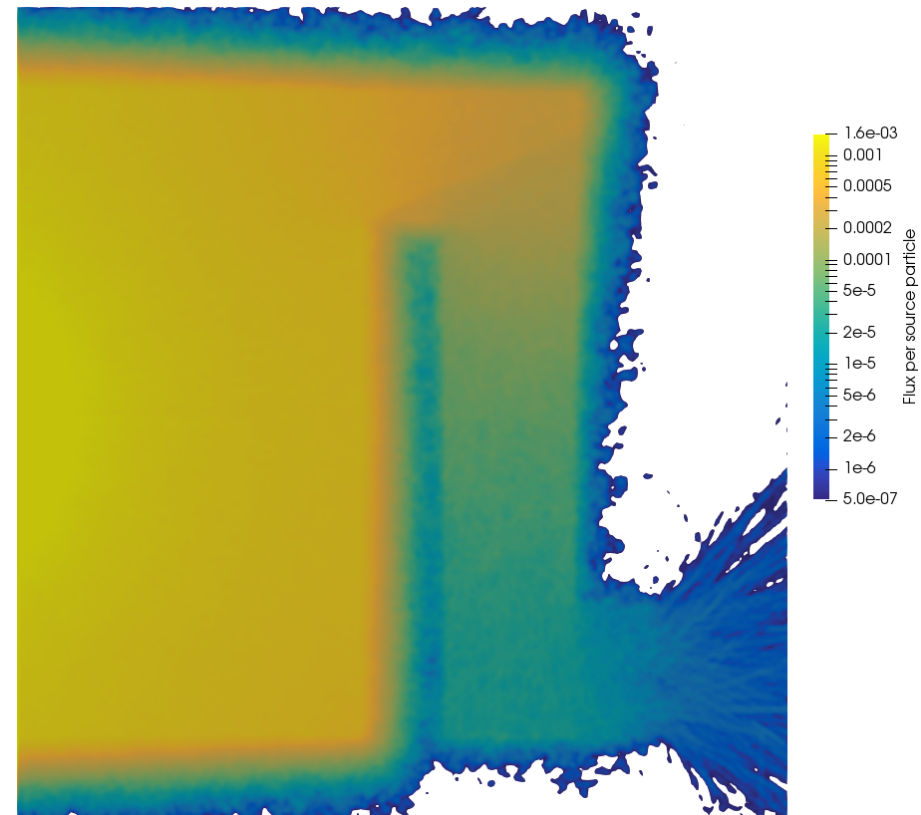
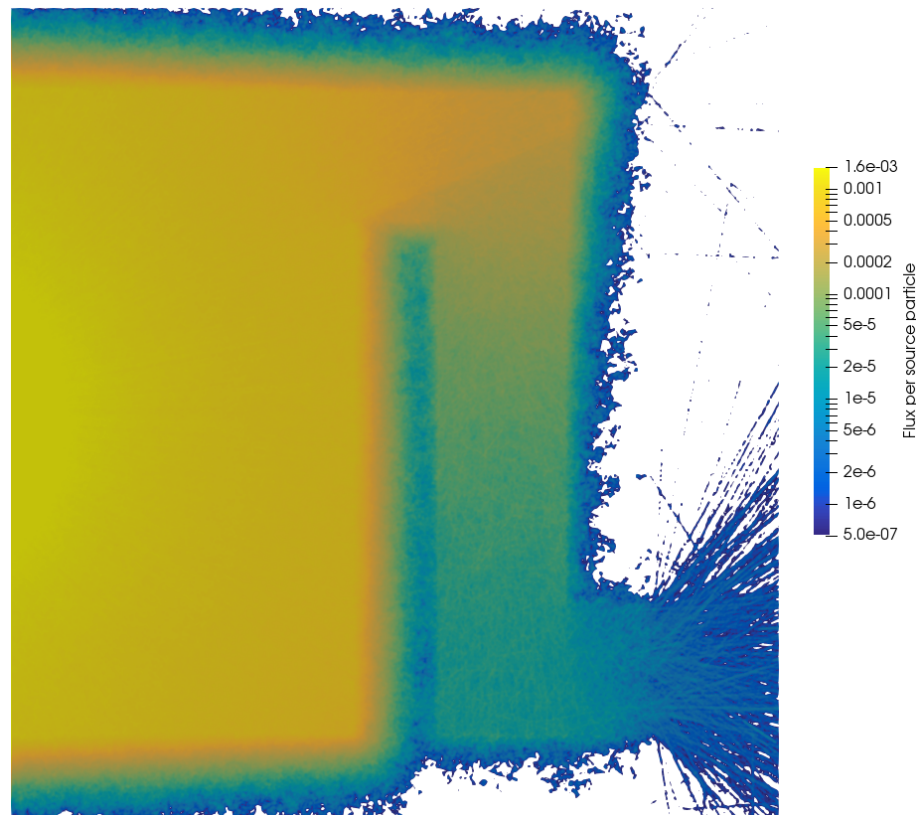
- **XCP-3 POC: T. Burke**
- **Supports performing tallies on GPUs asynchronously with transport on CPUs**
- **Takes particle events and material information from a Monte Carlo code and performs a variety of tallies:**
 - Track-length estimator
 - Collision estimator
 - Surface-crossing flux estimator
 - Kernel density estimator (KDE)
 - Functional expansion tally (FET)
 - Sensitivity coefficients and derivatives
- **Intended for open-source distribution!**
- **T.P. BURKE, “Development of a Library for Conducting Monte Carlo Tallies on Heterogeneous Systems”, Los Alamos National Laboratory, LA-UR-27987 (2018).**

Kernel Density Estimators

- **Instead of each particle being represented at a point in space, each is given a bandwidth**
- **Thus, each particle can score to multiple tally points**
- **This smooths out the solution and reduces variance:**
 - The smoothing can introduce a bias; sharp gradients in the solution may be artificially flattened
 - Bias is proportional to the bandwidth
 - Variance is inversely proportional to the square of the bandwidth
- **Bandwidth is typically a function of mean free path**
- **KDEs are well suited for GPUs**
 - CPU does all the transport
 - Collision site information is transferred to the GPU (many collision sites are buffered and sent together)
 - The GPU can use many threads to score to many tally points without thread divergence

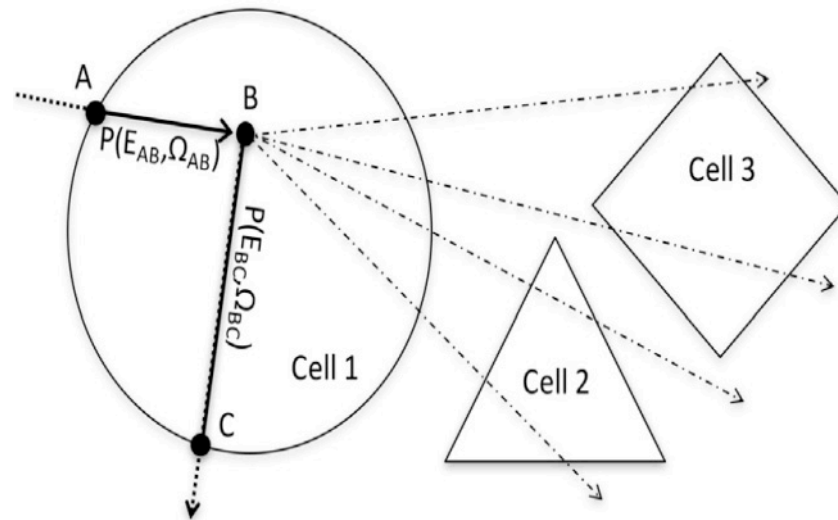
Kernel Density Estimator Results

Flux from a 1-MeV neutron point source in a concrete treatment room using mesh tallies (left) and KDE with a bandwidth of 5 cm and a delta-scattering cross section MFP of 0.5 cm (right).



Volumetric Ray-Casting Estimators

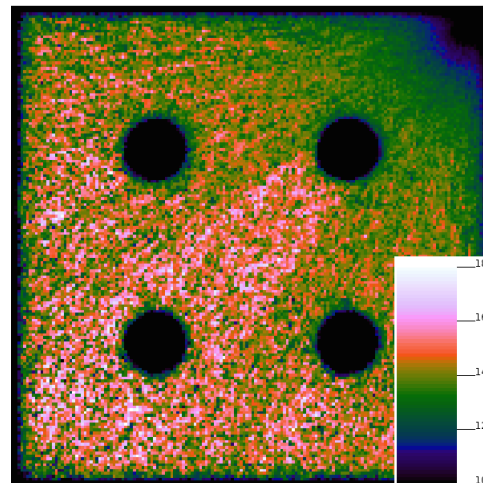
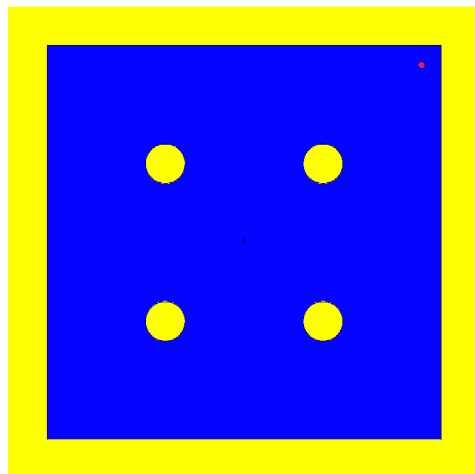
- Sample multiple pseudo-rays at each source and collision event and perform a ray trace to generate expected track-length contributions to volumetric tallies.
- These rays are transferred to the GPU (many rays are buffered and sent together)
- GPU then traces the rays through the geometry and scores to the tally
- Up to 16x improvement in performance vs. track-length tally on CPU



Volumetric Ray-Casting Estimator Results

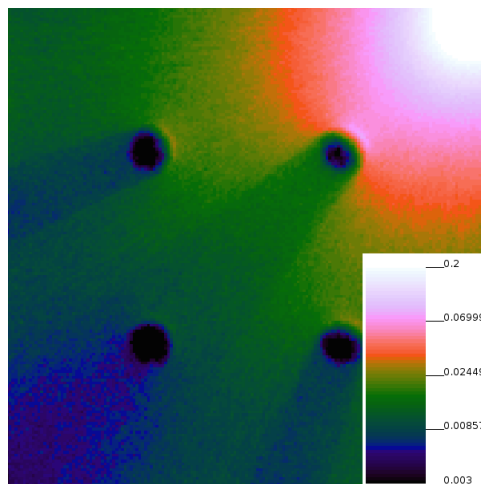
Performance of volumetric-ray-casting estimator for a room-sized shielding problem.

Geometry: U
Sphere in a
Concrete Room

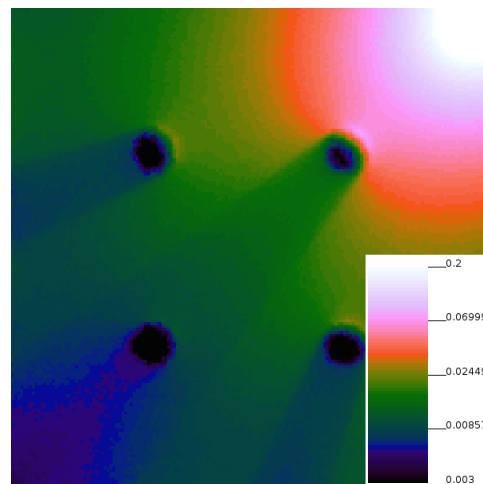


Relative
Performance of
GPU vs. 8 CPU
Cores

Standard Track-
Length Flux Tally



Ray-Casting Flux
Tally



Discussion

Summary

- **LANL has a long history of scientific computing and transport methods development**
- **We are still a leader in these fields**
- **We apply our knowledge to problems ranging from fundamental physics to all aspects of national security**

Student Project Ideas (a partial list)

- **V&V – Setup and run benchmark problems**
- **Stochastic systems analysis:**
 - Calculation of Feynman-Y moment and comparison to experiment
- **Transients with delayed neutrons**
 - Incorporate real delayed neutron data from ACE data files
 - Run all variants of C5G7-TD
- **GPU programming and performance optimization**
- **Functional expansion tallies for radiography**
- **Performance profiling of CPU coding**

Student Project Ideas (a partial list)

- Use AI to generate weight windows for well-defined classes of neutron and photon transport problems
- Investigate performance of track-length vs. expected value estimators
- Weight-window-like method to determine number of rays per collision for volumetric ray-casting estimator
- Demonstrate neutron and photon ray-tracing through unstructured mesh on Nvidia real-time ray tracing hardware
- Incorporate CERN's ROOT Monte Carlo Geometry into MCATK and/or MCNP
- Import/Export CERN's GDML for MCATK's solid body geometry
- Prototype a tally server
- Prototype a cross section server



Thank you!

Contact Info:
Travis Trahan
tjtrahan@lanl.gov